Supplementary data

for

Triazole-acetate functionalized gold nanoparticles for colorimetric Pb(II) sensing

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Contents

1. Synthesis of 5-(1,2-dithiolan-3-yl)-*N*-(prop-2-yn-1-yl)pentanamide (**TP**)[1]

DIEA (270mL, 1.55mmol), *O*-(benzotriazol-1-yl)-*N,N,N′,N′*-tetramethyluronium hexafluorophosphate HBTU (584mg, 1.55mmol) and propargylamine (106mL, 1.55mmol) were added to a suspension of (+/-) lipoic acid (212 mg, 1.03mmol) in 5 mL of CH_2Cl_2. The mixture was stirred overnight at room temperature, and then diluted with 10mL of CH_2Cl_2.The organic layer was separated, washed successively with water, 10% aqueous solution of citric acid and brine. The organic layer was then dried over Na_2SO_4, filtrated and evaporated to dryness. The crude material was purified by column chromatography (silica gel, dichloromethane:acetone, 10:1) to afford the product as a white powder (205 mg, 82%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.77 (s, 1H), 4.05-4.07 (m, 2H), 3.56-3.60 (m, 1H), 3.12-3.19 (m, 2H), 2.46-2.48 (m, 1H), 2.20-2.25 (m, 3H), 1.66-1.75 (m, 5H), 1.46-1.50 (m, 2H).

2. Synthesis of azidoacetic acid[2]

To a solution of sodium azide (820 mg, 12.6 mmol) in 4.2 mL of water, bromoacetic acid (1 g, 6.3 mmol) was slowly added. The solution was stirred at room temperature overnight. The reaction was then quenched by dropwise addition of 3.5 mL of conc. HCl (37%). After extraction with Et_2O (45 mL), the organic phase was dried over $MgSO_4$ and concentrated to afford azidoacetic acid as an oil (5.9 mmol, 94%). ^{1}HNMR (300 MHz, $CDCl_3$): δ 10.16 (1H, s, COOH), 3.97 (2H, s, CH_2). IR: 2108.45 cm^{-1}. MS (GC) m/z calcd for $C_2H_3N_3O_2$ 101.02, found 101.02.

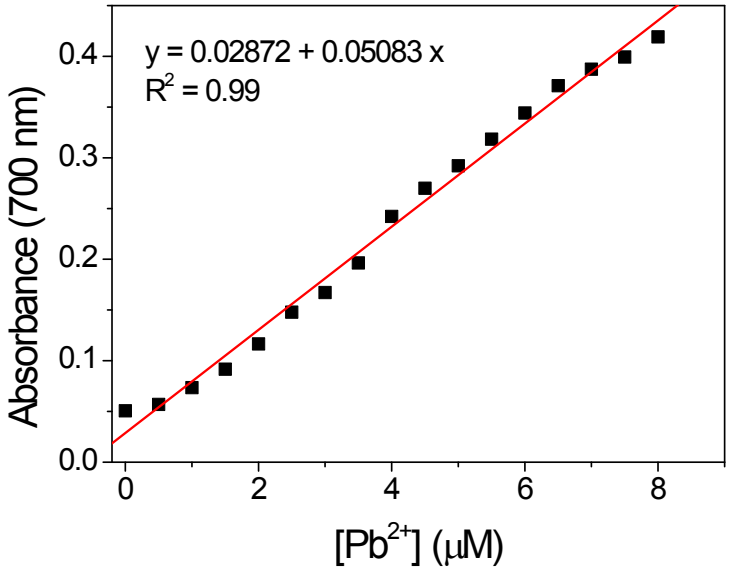

Figure S1. The calibration curve of TTA-AuNPs. The detection limit (DL) of **HCS** with HOCl was determined from the following equation: DL = K * S_b / S, where K = 3; S_b is the standard deviation of the blank solution; S is the slope of the calibration curve.

DL = 3 x 0.000283 / 0.05083 = 0.0167 (μM) = 16.7 nM

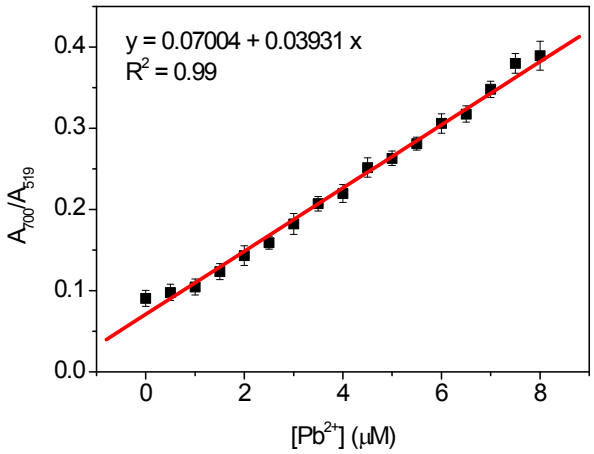

Fig. S2. The calibration curve for the detection of Pb^{2+} by TTA-AuNPs. The ratio (A_{700}/A_{519}) was plotted against different concentrations of Pb^{2+} ions.

Reference

1. D. Garin, F. Oukhatar, A. B. Mahon, A. C. Try, M. Dubois-Dauphin, F. M. Laferia, M. Demeunynck, M. M. Sallanon, S. Chierici, *Bioorg. Med. Chem. Lett.*, 2011, **21**, 2203-2206

2. N. Brabez, R. M. Lynch, L. Xu, R. J. Gillies, G. Chassaing, S. Lavielle, V. J. Hruby, *J. Med. Chem.*, 2011, **54**, 7375-7384.